

|   |  |                                 |                                 |                  |
|---|--|---------------------------------|---------------------------------|------------------|
| <b>Module Name</b>  |  | <b>Modul Code</b>               |                                 |                  |
| Introduction to Numerical Mathematics in Chemistry  |  | chem5014-01a                    |                                 |                  |
| <b>Module Coordinator</b>   |  |                                 |                                 |                  |
| Prof. Dr. Bernd Hartke  |  |                                 |                                 |                  |
| <b>Organizer</b>  |  |                                 |                                 |                  |
| Section Chemistry   |  |                                 |                                 |                  |
| <b>Faculty</b>  |  |                                 |                                 |                  |
| Faculty of Mathematics and Natural Science  |  |                                 |                                 |                  |
| <b>Examination Office</b>   |  |                                 |                                 |                  |
| Examination Office Chemistry  |  |                                 |                                 |                  |
| <b>ECTS Credits</b>   |  | 5                               |                                 |                  |
| <b>Evaluation</b>   |  | Graded                          |                                 |                  |
| <b>Duration</b>   |  | One Semester                    |                                 |                  |
| <b>Frequency</b>  |  | Annually Summer Semester        |                                 |                  |
| <b>Workload per ECTS Credit</b>   |  | 30 h                            |                                 |                  |
| <b>Total Workload</b>   |  | 150 h                           |                                 |                  |
| <b>Contact Time</b>   |  | 56 h                            |                                 |                  |
| <b>Independent Study</b>  |  | 94 h                            |                                 |                  |
| <b>Teaching Language</b>  |  | German / English                |                                 |                  |
| <b>Module Courses</b>   |  |                                 |                                 |                  |
| <b>Course Type</b>  | <b>Course Name</b>                                 | <b>Compulsory/<br/>Optional</b> | <b>SWS</b>                      |                  |
| Lecture   | Introduction to Numerical Mathematics in Chemistry | Compulsory                      | 2                               |                  |
| Practical Exercise  | Introduction to Numerical Mathematics in Chemistry | Compulsory                      | 2                               |                  |
| <b>Examination(s)</b>   |  |                                 |                                 |                  |
| <b>Examination Name</b>   | <b>Type of Examination</b>                         | <b>Evaluation</b>               | <b>Compulsory/<br/>Optional</b> | <b>Weighting</b> |
| Examination: Introduction to Computational Chemistry  | Other  | Graded                          | Compulsory                      | 100              |
| <b>Further Information on the Examination(s)</b>  |  |                                 |                                 |                  |
| <ul style="list-style-type: none"> <li>Exams: for each chapter, programs are handed in, checked and graded,</li> <li>Exam language: English or German (selected by student).</li> </ul> |  |                                 |                                 |                  |
| <b>Course Content</b>   |  |                                 |                                 |                  |
| <ul style="list-style-type: none"> <li>Crash course computer programming: Fortran,</li> <li>Integration: Euler, Simpson, Gauß,</li> </ul>   |  |                                 |                                 |                  |

- Random numbers and Monte-Carlo algorithms,
- Ordinary differential equations: Euler, Runge-Kutta,
- Systems of differential equations,
- Systems of linear equations, matrix inversion,
- Linear and non-linear regression, Spline interpolation,
- Matrix diagonalization: Jacobi,
- Root search: bisection, Newton.

### Learning Outcome

- Basic introduction to numerical methods and their computer implementation, selected for their usefulness in chemistry,
- understanding fundamental principles of numerical calculations,
- ability to program and use simple numerical methods,
- ability to select and use appropriate library routines,
- tests and critical appreciation of numerical results.

### Reading List

- Press/Flannery/Teukolsky/Vetterling: „Numerical Recipes“, Cambridge,
- Stoer/Bulirsch: „Numerische Mathematik 1,2“, Springer,
- Deuffhard et al.: „Numerische Mathematik 1,2,3“, de Gruyter, lecturer's scriptum.

| Use   | Compulsory/<br>Optional | Semester  |
|---|-------------------------|-----------|
| Master, 1-Subject, Chemistry, (Version 2016)            | Optional                | 1, 2 or 3 |
| Bachelor, 1-Subject, Business Chemistry, (Version 2014) | Optional                | 6         |
| Bachelor, 1-Subject, Business Chemistry, (Version 2017) | Optional                | 6         |
| Master, 1-Subject, Business Chemistry, (Version 2014)   | Optional                | 1 or 2    |
| Master, 1-Subject, Business Chemistry, (Version 2017)   | Optional                | 1 or 2    |